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Dissertation outline

Chapter 1 Introduction

Energy is the most essential resource for humankind's progress, evolution and prosperity. This chapter tries to provide the definition of energy, and the importance of energy for human societies. The effects of overuse of fossil fuels on the environment will be briefly described. From these effects, the driven force of encouraging people to use sustainable energy appears. After explaining the superiority of photovoltaics which could lead it much more popular than other kinds of sustainable energy, as well as, the history of solar cells' development, most significantly, the character of this dissertation, a new fantastic group of solar cells, perovskite solar cells will be introduced here.

Chapter 2 A mini review on carbon nanotubes electrode based hole conductor free perovskite solar cell

In this chapter, a brief review of carbon materials based hole-conductor-free perovskite solar cells (C-PSCs) will be presented in particular interests. In the recent few years, perovskite solar cells (PSCs) gain so much attention from both scientific community and commercial field because of its high-power conversion efficiency and relative low-cost production process, which is associated with a simply solution fabrication technique, comparing with current commercial solar cell such as crystalline Si and CIS solar cells. However, before PSCs go to commercialization, it still has a long way to go to overcome the stability and scaling up problems. In PSCs, the metal electrode and hole-transport-material (HTM) are blamed as resources of its degradation. Therefore, carbon-based materials with their excellent charge transfer characteristics and water-resistant are expected to be the best candidate to replace both novel metal electrode and HTM. After explaining the motivation of developing this type of PSCs, the device physical structure and its working principles of this group of PSCs will be introduced. The progress of development of carbon nanotube based hole transport material free perovskite solar cells (CNT-based HTM-free PSCs) will be also summarized in this chapter.

Chapter 3 Impacts of structure defects and carboxyl and carbonyl functional groups on the work function of multi-walled carbon nanotubes

The work function is important for achieving the desired performance of many electronic devices. Several investigations have been conducted on the work-function engineering of multi-walled carbon nanotubes (MWNTs). Oxidation of carbon nanomaterials is a simple approach to increasing MWNTs' work function without introducing extrinsic metallic elements or altering the nanotubes' morphology; however, few experiments have been conducted to study the mechanism by which different types of oxygen-containing functional groups increase the work function of MWNTs. In this chapter, I designed and carried out systematic experiments to investigate the influence of the overall oxygen content, structure disorder, and two individual types of functional groups on work-function shifts. Our results demonstrate that the work function is not simply correlated with the overall oxygen concentration, that structure defects are unlikely to change the work function, and that carbonyl groups are the dominant contributor to the increase in the work function of MWNTs. Our results provide distinctive insights into work-function engineering of MWNTs and guide the application of MWNTs in functional devices for photovoltaic and optoelectronic devices.

Chapter 4 The crystallization and morphologies of perovskite absorber

The crystallization and the stability of organic-inorganic perovskite material ($\text{CH}_3\text{NH}_3\text{PbI}_3$) will be discussed in this chapter. The strategies of forming perovskite absorber layer are described, the different fabrication methods resulting in different crystal morphologies will be shown in this chapter as well. Since carbon nanotube as a fantastic candidate to replace metal electrode and eliminate hole-transport-material, the effects of capping carbon nanotube on PbI_2 and further influence on perovskite crystallization will be studied.

Chapter 5 Work function tailored multi-walled carbon nanotubes as a bifunctional material in perovskite solar cells

In this chapter, a better performance is expected by choosing a carbon nanotube with a tailored work function to optimize the charge transfer, electrode coverage and energy alignment in hole-transport-material-free perovskite solar cell. The effects of carbon nanotube electrode from functional groups, coverage and work function on the critical parameters of hole-transport-material-free perovskite solar cell (i.e. the open circuit voltage, short circuit current, the interface charge transfer characteristics etc.) would be investigated. In previous chapter, the mechanism of work function changing by simple oxidation treatment or nitrogen doping in carbon nanotube has been elucidated, which indicates a pathway to modify the work function to suit hole-transport-material-free perovskite solar cell's energy alignment better. More importantly, providing us a pathway to study the junction formation perovskite absorber and carbon nanotube, as well as, the functional groups effect on charge transfer through the interface of perovskite absorber and carbon nanotube. The coverage differences from different functionalized carbon nanotube are also studies to eliminate the performance difference from the external factor. A carbon nanotube based hole-transport-material-free perovskite solar cell's fabrication method is established and cells performances close to the current highest efficiency with a similar structure by applying the suitable carbon nanotube.

Chapter 6 Conclusions and outlooks

In this dissertation, low cost carbon nanotube-based hole transport material-free perovskite solar cells with high efficiency have been fabricated. In order to achieve a promising performance, lifting up the work function of carbon nanotube could be an effective strategy since the original work function of carbon nanotube is too close to the conduction band of perovskite absorber leading to serious back electron transfer process which hinders the device to achieve a promising performance. Thus, an easy and effective way of changing carbon nanotubes' work function but without changing carbon nanotubes' excellent intrinsic properties is necessary. Additionally, the side effects from increasing work function of carbon nanotubes on charge transfer or perovskite solar cell performance should also be investigated to clarify or indicating the right principle of work function engineering for all the carbon-based perovskite solar cell.